

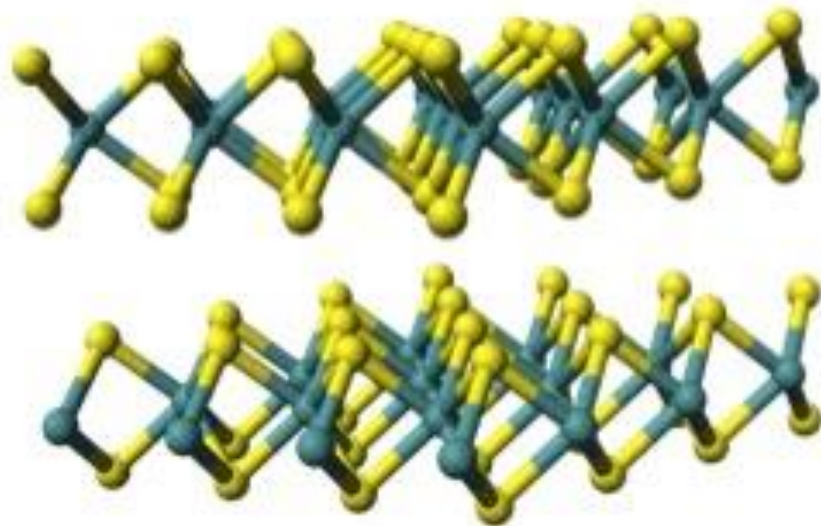
Center for the Computational Design of Functional Layered Materials (CCDM)

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EFRC mission statement

To develop, apply, and validate methods to calculate the electronic structure of materials. While these methods can be useful for the design of many new materials, we focus on the layered and two-dimensional materials that have potential for clean-energy technologies.

<http://efrc.cst.temple.edu>



RESEARCH PLAN

We are developing efficient and accurate density functionals including intermediate or full-range van der Waals interaction, and higher-level methods. These methods are being applied to understand how properties of layered materials are affected by composition, structure, defects, interfaces, and strain, and to the catalysis of hydrogen evolution.